

# Quantum Dot Version of Berry's Phase: Half-Integer Orbital Angular Momenta

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We show that Berry's geometrical (topological) phase for circular quantum dots with an odd number of electrons is equal to  $\pi$  and that eigenvalues of the orbital angular momentum run over half-integer values. The non-zero value of the Berry's phase is provided by axial symmetry and two-dimensionality of the system. Its particular value ( $\pi$ ) is fixed by the Pauli exclusion principle. Our conclusions agree with the experimental results of T. Schmidt *et al*, Phys. Rev. B **51**, 5570 (1995), which can be considered as the first experimental evidence for the existence of a new realization of Berry's phase and half-integer values of the orbital angular momentum in a system of an odd number of electrons in circular quantum dots.

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It is known for a long time already [1, 2], see also [3], that in certain cases half-integer quantization of the orbital angular momentum occurs in molecules. In Ref. [2] half-integer values of the orbital angular momentum are associated with the Berry's geometrical phase  $\pi$  that the nuclear wave function acquires under a pseudo-rotation around the equilateral configuration of the molecule  $\text{Na}_3$ . This was apparently the first experimental verification of the Berry's phase in high-resolution molecular spectroscopy. For reviews on Berry's phase [4, 5] in more general context see Refs. [6, 7].

In this paper we show that the half-integer quantization of the orbital angular momentum may occur also in circular quantum dots with odd numbers of electrons. In these systems the electron motion may be considered as being restricted to two dimensions. An assumption of axial symmetry of the confining potential ascertains the existence of loops that are not deformable to a point: the topology of the system is equivalent to that of a once-punctured plane. Hence there exists a topological Berry's phase. Since the Berry's phase defines a one-parametric set of self-adjoint generators of rotations, it determines the rotational dynamics of the electronic system, cf. [8]. The particular value of the Berry's phase follows from the Pauli exclusion principle. In circular quantum dots with

an odd number of electrons the Berry's phase takes the value  $\pi$  (similarly to the case of the sodium trimer [2]). Below we demonstrate that our conclusions agree with experimental results [9]. Based on our analysis presented in this paper, we believe that Ref. [9] may be considered as an observation of the new realization of the Berry's phase.

According to [10] (see also [11]) the oscillatory model with the parabolic confinement

$$V_{cf} = \sum_{a=1}^N m_* \Omega^2 \mathbf{r}_a^2 / 2 + V^{(0)}, \quad (1)$$

is a good approximation for low-lying levels in real circular  $N$ -electron quantum dots [12, 13]. Here  $m_*$  is the effective mass,  $\mathbf{r}_a$  is the two-dimensional coordinate of an electron, and the effective confining frequency  $\Omega$  and the reference energy level  $V^{(0)}$  are phenomenological parameters. In general  $\Omega$  and  $V^{(0)}$  depend on the number of particles in a quantum dot (cf. Ref. [10]) and the quantum numbers describing the state of the electronic system. Within this approach the Schrödinger equation can be written in dimensionless variables as

$$\left\{ -\frac{1}{4Q^2} \sum_{a=1}^N \frac{\partial^2}{\partial \boldsymbol{\rho}^2} + \sum_{a=1}^N \rho_a^2 + \frac{1}{2} \sum_{a \neq b}^N |\boldsymbol{\rho}_a - \boldsymbol{\rho}_b|^{-1} \right\} \Psi_N = \varepsilon(N) \Psi_N. \quad (2)$$

Here,

$$Q = \frac{1}{\hbar} \left( \frac{m_* e^4}{2\epsilon^2 \Omega} \right)^{1/3} = \left( \frac{\mu}{\epsilon^2} \right)^{1/3} \left( \frac{E_B}{\hbar \Omega} \right)^{1/3} \quad (3)$$

is the dimensionless parameter [14] which is determined

by the ratio of the characteristic Coulomb energy of electron-electron interaction to the mean level spacing in the confining potential. We employ the following notations:  $\epsilon$  is the effective dielectric constant,  $\mu = m_*/m_e$ ,  $a_B$  is the Bohr radius,  $E_B = m_e e^4 / 2\hbar^2$ ,  $-e$  and  $m_e$  are

charge and mass of a bare electron. The reduced energy  $\varepsilon(N) = [E(N) - V^{(0)}(N)]/E_0$  and the dimensionless coordinate  $\rho_a = \mathbf{r}_a/a_0$  are determined by the characteristic energy and the characteristic size of the system

$$E_0 = Q\hbar\Omega = \frac{\mu E_B}{\epsilon^2 Q^2}, \quad a_0 = \left( \frac{2e^2}{\epsilon m_* \Omega^2} \right)^{\frac{1}{3}} = \frac{2\epsilon}{\mu} Q^2 a_B. \quad (4)$$

Formally, Eq. (2) is equivalent to the Schrödinger equation for  $N$  particles with the mass  $2Q^2$ . In the classical limit  $Q \rightarrow \infty$  it determines the equilibrium configuration of electrons corresponding to the minimum of the potential energy. For example, in a three-electron quantum dot the electrons would be located at the vertices of an equilateral triangle at the distance  $\rho_0 = (2\sqrt{3})^{-1/3}$  off its center. The corresponding reduced energy is  $\varepsilon_{cl}(3) = 3\sqrt{3}/2\rho_0$ . For finite  $Q$  corrections to  $\varepsilon_{cl}(3)$  (harmonic and anharmonic) may be calculated by means of the  $1/Q$ -expansion [15]. For the first three terms of the  $1/Q$ -expansion for the energy of the ground state of a three-electron quantum dot we have [15]

$$\varepsilon_M(3) = 3.9311 + 3.0908Q^{-1} + (0.1908M^2 + 0.0284)Q^{-2}, \quad (5)$$

where  $M$  is an eigenvalue of generator of rotations  $\hat{L} = -i\partial/\partial\varphi$ ,  $\varphi$  is the angle of rotation of the system as a whole,  $0 \leq \varphi < 2\pi$ .

It is well known that the differential operator  $\hat{L}$  becomes self-adjoint, i.e. determines an observable, if it is defined on the Hilbert space of wave functions obeying boundary conditions, which in their most general form read [8],

$$\Psi(2\pi) = e^{i\theta}\Psi(0), \quad 0 \leq \theta < 2\pi, \quad (6)$$

(see also a recent paper [16]). The phase  $\theta$  arising as a result of rotation of the system around the axis of symmetry by  $2\pi$  may be called the Berry's geometrical (topological) phase. Usually, the Berry's phase [4, 5] is acquired by a wave function in the process of evolution of a system determined by a Hamiltonian. Here the topological phase  $\theta$  itself determines an operator  $\hat{L}_\theta$  from a one-parameter family of self-adjoint operators and hence the unitary operator  $\hat{U}_\theta$  which describes the rotational dynamics of the system similarly to the evolution operator,

$$\Psi(\varphi + \tau) = \hat{U}_\theta(\tau)\Psi(\varphi) = \exp(i\tau\hat{L}_\theta)\Psi(\varphi).$$

In virtue of Eq. (6), the eigenvalues of the generator  $\hat{L}_\theta$  are given by

$$M = \gamma + m, \quad m = 0, \pm 1, \dots, \quad \theta = 2\pi\gamma, \quad 0 \leq \gamma < 1. \quad (7)$$

The corresponding eigenfunctions

$$\Psi_M(\varphi) = \exp(iM\varphi)/\sqrt{2\pi} \quad (8)$$

implement an irreducible representation of the two-dimensional rotation group.

Due to axial symmetry, the wave functions in our problem are not eigenfunctions of the 3D angular momentum operator but of only its projection (represented by  $\hat{L}_\theta$ ) on the axis of rotation. Hence, according to (7)  $\gamma$  is in principle an arbitrary number, compare, e.g., [1]. Its specific value is determined by additional physical reasons. If we require that the wave function remains unaltered after the rotation of the system by  $2\pi$ , then  $\gamma = 0$  and the eigenfunctions (8) implement a single-valued representation of  $O(2)$ . In this case the orbital angular momentum eigenvalues are (up to the factor of  $\hbar$ ) integers. In cases where  $\gamma$  is a rational number the representation is multiple-valued and the momentum quantization may be fractional. However, if the system is invariant with respect to time inversion, only two cases  $\gamma = 0$  or  $\gamma = 1/2$  can be realized [16].

We now go back to the problem (2) with the odd number of electrons  $N$ . Consider first the case  $Q \rightarrow \infty$ . The ground state is realized by a rigid configuration of electrons minimizing the potential energy. This state is invariant under the  $2\pi$  rotation around the symmetry axis. This may be used to understand the quantization of the angular momentum operator. Indeed, the overall phase acquired by the ground state wave function after the rotation is determined by the total momentum  $J$ . The  $2\pi$  rotation of a two-dimensional system is obviously the identity element of the symmetric group  $S_N$  and thus belongs to the alternating group  $A_N$  of even permutations of the set  $\{1, \dots, N\}$ . Hence, the  $2\pi$  rotation of the system is equivalent to an even number of pairwise transpositions, and according to the Pauli exclusion principle the wave function do not change:

$$\exp(i2\pi J) = 1, \quad J = M + \Sigma = 0, \pm 1, \pm 2, \dots \quad (9)$$

Here the total momentum  $J$  is represented by the sum of the orbital and spin angular momenta. Since the number of electrons is odd, the spin quantum number  $\Sigma$  is half-integer. Thus the orbital angular momentum  $M$  must also take a half-integer value. According to Eq. (7) this implies that  $\gamma = 1/2$  or that the system is characterized by the Berry's phase  $\pi$ . To arrive to this conclusion we have considered the classical limit  $Q \rightarrow \infty$ . However, if one varies the parameter  $Q$  adiabatically, the quantum numbers  $M$  and  $\Sigma$  cannot change. Therefore our result is valid also at  $Q \sim 1$  which is typical for real quantum dots.

Consider now the case of three electrons. If the total spin number  $\Sigma = \pm 1/2$ , then  $M$  can take any half-integer value. However, the situation is different if  $\Sigma = \pm 3/2$ . Then there is an additional symmetry in the problem. The symmetry group of such system is  $C_{3v}$  which is isomorphic to the symmetric group  $S_3$ . The group  $C_{3v}$  consists of rotations about the symmetry axis by multiples of the angle  $2\pi/3$  (the  $C_3$  group) and reflections in the three bisectrices of the triangle.  $C_3$  is isomorphic to  $A_3$  and thus the wave function of the system at  $Q \rightarrow \infty$  does

not change also if it is subjected to a rotation by  $2\pi/3$ . Thus,

$$\exp(iJ2\pi/3) = 1, \quad J = M + \Sigma = 0, \pm 3, \pm 6, \dots \quad (10)$$

This means that  $M$  can take the values  $M = \pm(3+6k)/2$ ,  $k = 0, 1, 2, \dots$

Now we show that our conclusions are in excellent agreement with the experiment of T. Schmidt *et al.* [9]. The authors of Ref. [9] measured the ground state energy  $E(N)$  of  $N$ -electron circular quantum dots in GaAs-based heterostructures in a perpendicular magnetic field  $0 \leq H \leq 16 T$  for  $N = 1 \div 30$ . To explain the data, we should modify the calculation of the spectrum of a quantum dot in order to take into account the magnetic field [17]. For this purpose it is enough to make the changes in Eqs. (2)-(4): (i)  $\Omega(N) \rightarrow \Omega_L(N)$ , where  $\Omega_L = \sqrt{\Omega^2 + \omega_L^2}$  and  $\omega_L = eH/2m_*c$  is Larmor frequency; (ii)  $Q \rightarrow Q_L = (\mu/\epsilon^2)^{1/3}(E_B/\hbar\Omega_L)^{1/3}$ ; and (iii) take into account the Zeeman shift. This way we find for the energy of a quantum dot

$$E_{M\Sigma}(N; H) = \varepsilon_M(N; H)Q_L\hbar\Omega_L(N) \quad (11)$$

$$-(M + \mu g \Sigma)\hbar\omega_L + V_{M\Sigma}^{(0)}(N),$$

where  $g$  is the effective Lande factor and  $\varepsilon_M(N; H)$  replaces  $\varepsilon_M(N)$  in Eq. (2) after the change  $Q \rightarrow Q_L$ . The first three terms of  $1/Q$ -expansion for  $\varepsilon_M(3; H)$  are given by Eq. (5) with  $Q$  replaced by  $Q_L$ .

It is very important that the first term in the RHS of Eq. (11) depends on  $H^2$ . Therefore, in a weak field,  $\omega_L \ll \Omega(3)$ , the derivative of energy with respect to magnetic field is determined for the most part by the Zeeman energy

$$\left. \frac{dE_{M\Sigma}}{dH} \right|_{H=0} = -\frac{e\hbar}{2m_*c}(M + \mu g \Sigma), \quad (12)$$

and does not depend on the shape and parameters of the confining potential. In the experiment [9] the typical values of the parameters are  $\epsilon = 12.5$ ,  $\mu = 0.067$ , and  $g = 0.44$ . Thus the coefficient in the RHS of Eq. (12) is equal to 0.864 (measuring  $E_{M\Sigma}$  in  $meV$  and  $H$  in  $T$ ). On can see from Eq. (11) that at  $H \approx 0.5T$  the quadratic term in the expansion of  $E_{M\Sigma}$  becomes of the order of the Zeeman energy. Therefore the weak-field interval is  $0 \leq H < 0.5T$ .

We calculate the effective Coulomb energy  $E(3, H) - 3E(1, H)$  which was measured in the experiment [9] and show its weak-field dependence (dashed line) in Fig. 1. For the energy of a one-electron quantum dot we adopt the expression  $E(1, H) = \hbar\Omega_L(1) - \mu g \hbar\omega_L/2$ , where  $\hbar\Omega_L(1)$  is Fock-Darwin energy and  $\hbar\Omega(1) = 3.60 meV$  [9]. The experimental points are taken from Ref. [9]. The diameter of the circles corresponds to the size of experimental points in Fig. 3 of Ref. [9] and reflects experimental error of approximately  $0.025 meV$ . Two other

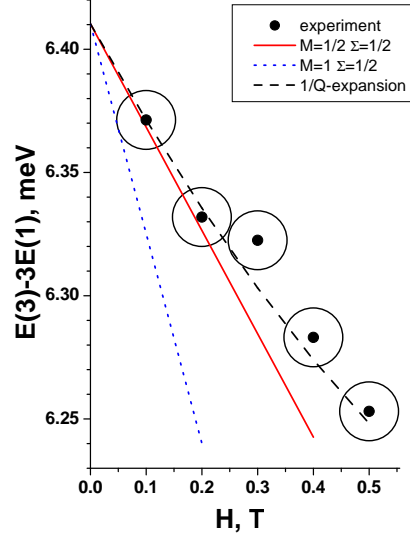


FIG. 1: The effective Coulomb energy  $E(3) - 3E(1)$  versus magnetic field  $H$  for weak field,  $\omega_L \ll \Omega(3)$ . The dashed line gives the results of calculations according to Eq. (11) in approximation (5) with parameters  $\hbar\Omega(3) = 4.69 meV$ ,  $V^{(0)}(3) = -17.44 meV$  and  $\hbar\Omega(1) = 3.60 meV$ . The experimental points are taken from Ref. [9]. The size of the circles corresponds to the size of experimental points in Fig. 3 of Ref. [9] and reflects experimental error of approximately  $0.025 meV$ . The solid and the dashed lines shows the slope of  $E(3, H) - 3E(1, H)$  at  $H \rightarrow 0$  calculated according to Eq. (12) for  $M = 1/2$  and  $M = 1$  respectively.

lines in Fig. 1 show the slope of  $E(3, H) - 3E(1, H)$  at  $H \rightarrow 0$  calculated according to Eq. (12). For the solid line  $M = 1/2$  and for the dotted one  $M = 1$ . It is clear from Fig. 1 that, unlike the value  $M = 1$  for the orbital angular momentum considered by the authors of Ref. [9], the value  $M = 1/2$  agrees with the data quite well. Deviation of experimental points from the linear law (12) at  $H > 0.2 T$  is explained by influence of the quadratic term in the weak field expansion of  $E_{M\Sigma}$ .

The agreement between the data and our calculations leads us to believe that the results of the experiment [9] unambiguously specify the quantum numbers of the ground state of a three-electron quantum dot right up to the point of the first crossing, or up to such value of magnetic field  $H^{(cr)}$  when the symmetry of the ground state is changed [18]. Quantum numbers of the ground state after the first crossing cannot be chosen *a priori* because of the unknown dependence of the phenomenological parameters  $\Omega$  and  $V^{(0)}$  in Eq. (1) on the quantum numbers. Varying these parameters we can obtain an excellent fit of the experimental data [9] by the results of the  $1/Q$ -expansion. Certainly, in the experiment [9]  $Q \sim 1$ , or are even slightly less than 1. However, it was shown in

Ref. [15] that for the case of two-electron dots the first three terms of  $1/Q$ -expansion provide 3%-accuracy even at  $Q \lesssim 1$ . Since the relative contribution of the Coulomb repulsion for three-electron quantum dots is greater than for two-electron dots, we believe that the accuracy of approximation (5) in the region  $Q \sim 1$  is at least of the same order.

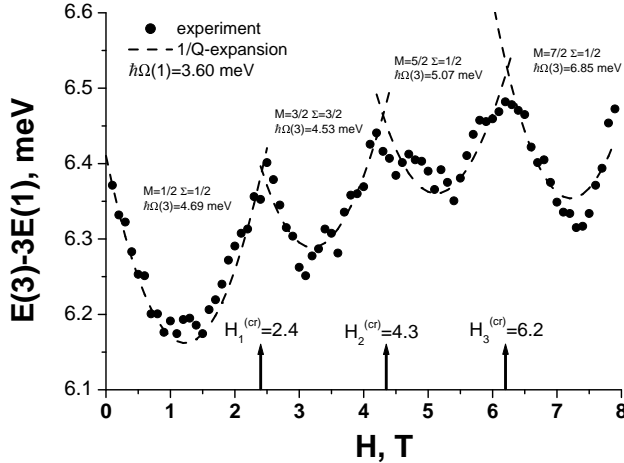


FIG. 2: Comparison of the experimental data (solid circles) of T. Schmidt *et al.* [9] for  $E(3) - 3E(1)$  with the results of calculations according to Eq. (11) in approximation (5). The numbers give the values of the total electron spin and orbital angular momenta, and the effective confining frequencies. Arrows indicate the crossing points.

The result of the fitting procedure is shown in Fig. 2. The experimental points are taken from Ref. [9]. We have found the locations of three crossings in the range  $0 < H < 8T$  at  $H_1^{(cr)} = 2.4T$ ,  $H_2^{(cr)} = 4.3T$  and  $H_3^{(cr)} = 6.2T$ . Quantum numbers  $M$  and  $\Sigma$  are chosen according to condition (9) everywhere except the region between the second and the third crossings,  $H_2^{(cr)} < H < H_3^{(cr)}$ , where condition (10) was used. The values of effective confining frequencies  $\hbar\Omega(3)$  are given in Fig. 2, and the values of the parameter  $V^{(0)}(3)$  in *meV* for successive intervals between the crossing points are  $-17.44, -16.23, -20.23, -35.81$ . One can see that the theoretical curve is in a very good agreement with the experiment.

We believe that the results shown in Figs. 1, 2 represent convincing evidence in favor of our interpretation of the experiment [9]. Therefore, we regard the data presented in Ref. [9] as the first experimental demonstration of the existence of theoretically admissible half-integer values of the orbital angular momentum in two-dimensional quantum systems. We are also inclined to believe that the

appearance of the Berry's phase  $\pi$  and half-integer quantization of the angular momentum in the experiment [2] arise due to exactly the same physical reasons as in the case of two-dimensional circular quantum dots. This is explained by the fact that the configuration of molecule  $\text{Na}_3$  (sodium trimer) considered in Ref. [2] coincides with the configuration of the system of three electrons in a quantum dot at  $Q \gg 1$  when all electrons are located in the vertices of an equilateral triangle.

In conclusion, we have predicted the existence of a new version of Berry's phase along with half-integer quantization of the orbital angular momentum for 2D axially symmetric systems with an odd number of confined electrons. We argue that the experimental data for circular quantum dots in a strong magnetic field [9] is in agreement with this statement.

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